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The coupling of protein dynamics to function, the case of myoglobin

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Protein function is a multi-step kinetic process, which, apart from chemical modification, requires the transfer a substrate molecule across the protein-solvent interface, further intramolecular displacements and ligand binding. Each of these steps depends on structural rearrangements of the transient substrate environment provided by the solvent, the protein matrix and the active site. With myoglobin the kinetics of ligand binding can be monitored in such detail with time-resolved optical spectroscopy, x-ray scattering and simulations. Moreover fast structural dynamics of myoglobin, its hydration shell and the heme active site have been probed by inelastic neutron scattering and Moessbauer spectroscopy. In this lecture I will show that two classes of structural motions and correlated kinetic steps can be discriminated from their susceptibility to the external solvent viscosity. The concept of the protein dynamical transition allows to integrate these features. There are neither masters nor slaves. Even small globular proteins can establish a reactive zone, which is both chemically and dynamically isolated from the solvent.

Literature: W. Doster, BBA Proteins and Proteomics (2010) 1804, 3-14.